

Progress In Multigroup Ion Transport Using MCNP

Noel Keen

University of New Mexico

Los Alamos National Laboratory (XTM)

noelk@unm.edu, ndk@lanl.gov

1 Introduction

This memo describes progress made in implementing low- and medium-energy ion transport in amorphous media using MCNP-4A[1]. MCNP has the capability for coupled multigroup photon and electron transport using the Boltzmann Fokker-Planck (BFP) formalism[2] with cross-section data generated by CEPXS[3]. This same formalism can be employed to transport any type of charged particle if the appropriate cross-section data are available. Minor changes (if any) are required to MCNP itself. A code called YATC has been developed to calculate the physics data needed for BFP ion transport. This method is now being validated in MCNP by comparisons with another ion transport code called TRIM[4].

2 Generating Ion Data (YATC)

YATC calculates the multigroup ion cross-section data required by MCNP. YATC is the result of several students' efforts over the past few years at the University of New Mexico[5]. The code is written in FORTRAN90 with efforts to maintain portability, readability and efficiency. A much more detailed explanation of the ion data generation and the BFP formalism can be found in reference [6].

There is work being done to allow YATC the ability to generate ion cross-section data for use with ONEBFP, which is a 1D discrete ordinates code. A parallel version of YATC is also being developed[7].

2.1 Charged Particle Interaction Physics

In this memo, the incident particle is referred to as the ion, and the particles comprising the target are called the target atoms. Two types of interactions are considered in the generation

of ion cross-section data: elastic scattering of the incident ion with the nuclear charge of the atom, and inelastic scattering of the ion with the atomic electrons of the target.

Elastic ion interactions are coupled in energy and angle; given an energy transfer, there is a corresponding scattering angle which is a result of momentum and energy conservation [8]. An interaction cross section is desired that can be expressed in terms of the incident energy and the scattering angle cosine only. YATC uses semi-empirical interatomic potentials to construct explicit expressions for the differential cross sections. The differential cross section used in this work is the Lindhard “magic formula”[9], which is an accurate one-parameter approximation given for two charged particles as:

$$\sigma(t) = \frac{\pi a^2}{2} \frac{f(t^{\frac{1}{2}})}{t^{3/2}} \text{ (cm}^2\text{)} \quad (1)$$

where

$$t = \left(\frac{E'}{E_L} \right)^2 \frac{(1 - \mu_{\text{CM}})}{2} \quad (2)$$

Here a , the screening radius, and E_L , the Lindhard reference energy, are both properties of a particular incident ion and target atom. The parameter μ_{CM} is the cosine of the angle θ in the scattering plane using the center-of-mass system, and E' is the energy of the incident particle. The cross section must then be converted to a function of E' and μ_{CM} using conservation relations:

$$\begin{aligned} \sigma(E', \mu_{\text{CM}}) &= \frac{1}{2\pi} \sigma(t) \left| \frac{dt}{d\mu_{\text{CM}}} \right| \\ &= \frac{1}{4\pi} \left(\frac{E'}{E_L} \right)^2 \sigma(t(E', \mu_{\text{CM}})) \text{ (cm}^2\text{/ster)} \end{aligned} \quad (3)$$

Various expressions are available for the universal screening function $f(t^{\frac{1}{2}})$. One example is the Universal Potential model[9] used in this work.

For inelastic scattering involving the interactions between the incident ion and the target atomic electrons, it is assumed that the ion experiences a continuous energy loss without angular deflection. This mechanism is typically treated in transport models with the Continuous Slowing Down Approximation (CSDA), and is characterized by the electronic stopping power S_e . In MCNP, the energy of an ion traveling between interaction sites is reduced by an amount determined by the stopping power. The code for the electronic stopping power used in YATC is taken (at least temporarily) from the model for stopping power used in TRIM (described in Running Trim section).

2.2 BFP Formalism and PRF methodology

Because of the long range nature of the interatomic potential, the differential scattering cross section obtained is very forward-peaked (Figure 1). This prevents the use of the usual

Legendre expansion of the scattering kernel because of the singularity at μ_{CM} equal to 1.0. To circumvent this singularity, the Boltzmann Fokker-Planck (BFP) approach [10, 11] is used which involves the decomposition of the scattering kernel into two components: a “Boltzmann” piece, Σ_s^B , representing discrete large angle scattering, and a “Fokker-Planck” piece, Σ_s^{FP} , which considers small angle scattering. The resulting two scattering operators are then treated separately. The sum of the two pieces equals the total scattering cross section.

$$\Sigma_s^{\text{Total}} = \Sigma_s^{\text{Boltzmann}} + \Sigma_s^{\text{Fokker-Planck}} \quad (4)$$

YATC uses the Partial Range Fit (PRF) methodology [12] to perform the decomposition suggested above. A μ_{CM} cut-off (μ_{cut}) close to 1.0 is introduced which defines the partial range. Choosing a μ_{cut} is somewhat ad hoc and is currently determined by trial and error. For electron transport with CEPXS/MCNP, this value is set at 0.9, however for ion-target pairs with arbitrary mass ratios, it is desirable to let μ_{cut} be an input parameter. For values of μ_{CM} below μ_{cut} , the differential scattering cross section is “smooth” and a Legendre expansion is constructed to fit the cross section over the partial range. This partial range fit is then extrapolated to μ_{CM} equal to 1.0. To obtain Legendre moments over the full range, another Legendre expansion is constructed to fit the extrapolated PRF, which is referred to as the full-range fit. The full-range fit is non-singular and is used by YATC to obtain the data required by the Boltzmann scattering operator. The remaining singular part of the differential cross section is treated separately by a Fokker-Planck (FP) approximation. Two parameters are needed to characterize the FP operator: the momentum transfer cross section, α , and the restricted nuclear stopping power, S_n^r . The momentum transfer represents the angular dependence of the FP operator, while S_n^r represents the energy dependence.

YATC calculates three main quantities that are required for BFP transport. From the Boltzmann component of the scattering cross section (Σ_s^B), the group-to-group transfer coefficients are obtained, which are the Legendre moments of the non-singular full-range cross-section representation, averaged over the energy groups. This includes a pseudo-absorption coefficient that describes the loss of particles by scattering below the minimum energy in the group-to-group transfer calculations. This absorption coefficient is really the probability that an ion will scatter to a “dummy” group below the last group in the problem and is, therefore, calculated in the same way as the group-to-group transfers. Note that ions can only scatter down in energy groups (no up-scatter). Another quantity calculated by YATC is the momentum transfer coefficient which represents the angular dependence of Σ_s^{FP} , averaged over the energy group. The last quantity is the stopping power which is a sum of the electronic stopping power and the restricted nuclear stopping power.

$$S = S_n^r + S_e \quad (5)$$

The electronic stopping power represents the continuous energy loss described above, while the restricted nuclear stopping power contains the energy dependence of Σ_s^{FP} .

2.3 YAG

A graphical user interface named YAG has been written to view the Legendre polynomial fits to the exact cross section and to serve as an interface for YATC. The fits can be viewed on the monitor with the ability to interactively modify parameters such as ion-target pair, Legendre order, μ_{cut} , and tolerance. YAG is primarily useful in the choosing of the Legendre order and μ_{cut} for a problem, as these values are problem dependent and determined largely by trial and error.

2.4 YATC Input

The input to YATC (`input`) is outlined below and an example of this file is listed in Appendix A.

Ion-Target pair: Any ion can be used with any target atom. Currently, only single species problems can be handled and all targets are assumed to be amorphous.

Legendre Order: The order of the Legendre expansion over the full range of scattering.

PRF Order: The order of the Legendre expansion over the partial range of scattering. In the work described in this memo, these two Legendre orders (for full range and partial range expansions) are always equal.

PRF Cut-Off μ_{cut} : The cut-off angle for the PRF. Defines the partial range. The same value used for μ_{cut} in a YATC calculation must also be used in the MCNP simulation.

Energy Grid: The energy group boundaries. YATC can create both linear and log group structure given maximum and minimum energy values. Explicit group boundaries can also be specified in `input`.

Tolerance: The tolerance to be used for most of the adaptive quadrature integrations performed in the code. Currently, the tolerance is specified to define the maximum allowed relative error.

Screening Function: The screening function to be used in the differential scattering cross section. The Universal Screening Function[9] is used in all work discussed in this memo, but other options have been implemented.

2.5 YATC Output

YATC outputs three files: `crsrd.inp`, `yout.dtf`, and `yout`. The `crsrd.inp` file is discussed in the section entitled “Running CRSRD”. An example of `crsrd.inp` can be found in Appendix B. The `yout.dtf` file contains the real data and is written in a format called “DTF-format”. For this work, all of the values in the DTF-formatted file are macroscopic

with the atomic density of the target material being calculated within YATC. The `yout.dtf` file contains the following data:

- group-to-group transfer for each Legendre moment [1/cm]
- absorption cross section for each group [1/cm]
- total cross section for each group [1/cm]
- momentum transfer for each group [1/cm]
- stopping power for each group [MeV/cm]

An example `yout.dtf` for a very simple problem is listed in Appendix C. The `yout` file is output by YATC to help in debugging, looking at intermediate results, and viewing the results contained in `yout.dtf` in a more readable format. A slightly modified example of this file is included in Appendix D.

3 Running CRSRD

CRSRD[14] is the step between YATC and MCNP. The DTF-formatted file created by YATC (`yout.dtf`) is converted to an ACE-formatted file which can be used by MCNP. Most importantly, CRSRD converts the Legendre expansion of angular scattering to discrete angles using the Radau quadrature method[13].

The `crsrd.inp` file produced by YATC contains the input for the CRSRD code including information such as the group structure, Legendre order, particle type, etc. An explanation of the CRSRD input can be found in reference [14] which also serves as the manual for CRSRD. Below are notes concerning CRSRD input parameters used for creating ion data that are worth pointing out:

- YATC does not include the “ $2*\ell+1$ ” factor in the data (`i2lp1 = 0`)
- Particle type is “other”. (For example, with 101 groups: `iincp = 1 101 0`)
- Use Radau discrete angle treatment for ions (`iang = 2`)

The CRSRD manual mentioned above is intended for a version of CRSRD that was stripped of BFP options. There exists a patch to include the missing BFP options necessary for handling ion cross-section data[15]. This BFP patch will work with the latest version of CRSRD on the open CFS. There was a bug found in CRSRD concerning the multigroup BFP data and a fix for this bug is included in the BFP patch[15]. The CRSRD manual does not discuss the inclusion of some necessary input to `crsrd.inp` for BFP cross-section data. In order to maintain generality and handle multiple particle species, CRSRD (with the BFP

patch) requires the mass of the incident particle for each group. The following paragraph explains how to include these masses.

For Section 2 of the CRSRD input, there should be the word “energy” on one line followed by the energy group boundaries. The number of entries should be the number of groups plus one. The boundaries are to be in decreasing order, in units of MeV, and can be in free-field input. The CRSRD manual does not mention that immediately after the group boundaries in Section 2, there should be the atomic mass of the incident ion in each group. The number of entries should be equal to the number of groups and the masses should be entered in units of MeV. For one ion-target pair (i.e. one particle problem), all of these masses will be identical.

CRSRD requires the input deck, `crsrd.inp`, and the cross-section data file in DTF-format. Output from CRSRD includes a type 1 file in the ACE format (`ace.out`), a cross-section directory file (`xmdir`), and a diagnostics file `xsproc.out`. The `ace.out` file is used directly by MCNP. An example of this file is included in Appendix E. The diagnostics file could contain warning messages encountered during the execution of CRSRD. Many of the cross-section data files used as input to CRSRD in this work have resulted in numerous warnings printed to the diagnostics file. These warnings are not presently understood, but it has been suggested that some of the warnings could be spurious.

4 Running TRIM

TRIM (Transport of Ions in Matter) is an ion transport code that can be used to model planar (slab) geometries. TRIM is part of a group of programs called SRIM[4] (the Stopping and Range of Ions in Matter) and is the industry standard for ion transport. In this work, TRIM is used to compare 1D ion deposition profiles with those of MCNP, where an ion deposition profile is the final distribution of incident ions as a function of depth in the target material.

TRIM is written entirely in BASIC code and except for the calculation of the stopping powers, the source code is not available. It is written for PC’s and must be run under DOS. The TRIM manual states that ions are transported using a full quantum mechanical treatment of ion-atom collisions. It goes on to describe methods which are Monte Carlo in nature, but do not include ideas such as multigroup cross sections or a BFP treatment which are inherent in MCNP. Therefore, it is not clear how well the results from MCNP should match those of TRIM.

Although TRIM can only handle slab geometries, the ions are transported in three dimensions and the final positions of deposited ions are one form of output available. TRIM can also create and transport recoil ions and provide various output such as energy deposition, target damage, sputtering, ionization, and phonon production. It is hoped to soon obtain various results with MCNP besides ion deposition, and compare these results with TRIM.

5 Using READMG

READMG[16] is a utility used for viewing the multigroup cross-section data files in the ACE format. The original code has been converted to FORTRAN90 and slightly enhanced to show more information about the data.

Input for READMG is a type 1 ACE file, `ace.out` and the output has been split into four files: `info`, `p0`, `cosines`, and `secondary`. The `info` file contains formatted output presenting various parameters about the ZAID, contents of NXS and JXS array, energy group structure, groups masses, total cross section, absorption cross section, stopping power, momentum transfer, and special “edit” reactions. The `p0` file contains a labeled table of all the group transfers for the 0th order Legendre moments as well as the multiplicity for each incident group. The `cosines` file contains the angular distribution matrix for each group transfer. For the ion work presented, these distributions represent the collapsing of the Legendre moments above P0 into discrete scattering angles as calculated by CRSRD using the Radau quadrature treatment. If there are any secondary particles (such as photons or recoils), information about these particles would be in the file `secondary`. Examples of files `info`, `p0`, and `cosines` are included respectively as Appendices F, G, and H.

6 Running MCNP

In MCNP, multigroup electrons and ions are treated in the same way, that is to “masquerade” as neutrons. Reference [17] is a useful reference concerning the multigroup transport in MCNP. It appears that no major modification to the MCNP code is necessary for the treatment of ions. A discussion about the possible modifications that will be considered can be found in the section “Possible Modifications to MCNP”.

6.1 MCNP Input Deck

The MCNP geometry used to test the ion transport is a single material slab with many surfaces layered through the slab. Ions that are transmitted through the slab or backscattered are permitted and tallied. The slab is made thick enough so that very few particles are transmitted through the back face of the slab. The surfaces are all parallel and there are 50 such surfaces or layers in the modelled slabs. For most of the simulations performed thus far, the surfaces are spaced evenly apart. The atomic density used in the input deck is +1.0, because the cross-section data are macroscopic. This will result in a MCNP warning message of having cells with densities greater than 40 gram/cc, which can be ignored[15].

The incident particles are modelled as a thin beam source and given a direction along an axis perpendicular to all the slab surfaces in the problem. The multigroup option card, `mgopt`, is used in the MCNP input deck with a negative value for the number of groups. This implies “special” treatment for multigroup particles and also means that the source energy for the ions must be specified by group number. The source particles will have energies chosen

randomly from within the source group with an average source energy equal to the midpoint of the first group. In order to compare results with TRIM, which uses a single energy for all source ions, the group structure input to YATC is such that the first group (group number 1) has a very narrow width centered around the desired source energy. Incidentally, this is why the attached plots show the number of groups as 101 or 201 to indicate not only the exact number of groups, but also that a very small first group is used (which does not follow the log structure of the other groups).

An energy cut-off is used in the input deck for MCNP and is chosen to be the lower bound of the final group (lowest energy of cross-section data). If a continuous slowing down event causes the energy of the particle to decrease below the energy cut-off, then the history is terminated.

YATC does not yet provide “edit” cross sections such as ion deposition or energy deposition (similar to what CEPXS generates). Therefore an alternative method of tallying the ion deposition is used. Surface tallies are used to count the number of ions entering and exiting each surface by using the **F1** tally with the **C0** card to specify the direction bins to tally (forward and backward). A **mctal** file is created by MCNP which contains all of the tally information. By conservation of ions, the total number of ions deposited between two surfaces can be determined. An example of an input deck used with MCNP is listed in Appendix I.

6.2 READTALLY

For purposes of explaining, the term “bin” will be used to refer to the volume between two surfaces in the modeled slab. A utility code named READTALLY was written to read the **mctal** file produced by MCNP and output the ions deposited in each bin as a function of depth, where the depth of each bin is taken to be its midpoint. The output is written to a file in column format to facilitate plotting.

6.3 SABRINA

SABRINA [18] has been used to view the 3D trajectories and various interaction sites of the ions in the slab. SABRINA could prove to be a useful tool in understanding the movement of the ions particularly when we begin to look at real problems in three dimensions with multiple target materials.

6.4 Possible Modifications to MCNP

CEPXS and YATC both use an angle cut-off μ_{cut} as part of defining Boltzmann and Fokker-Planck components of the cross-section data. However, for CEPXS this angle cut-off for multigroup electrons is fixed at 0.9 and MCNP uses the same fixed 0.9 in the transport of the electrons. For ions with various incident to target atom mass ratios, it is desirable to

vary μ_{cut} as 0.9 may make the integrals over the Fokker-Planck region unnecessarily difficult. A temporary patch to MCNP was made to allow μ_{cut} to be an input parameter using the `rdum` array available in MCNP[15]. If necessary, a formal patch to MCNP will be made to allow this value to be included in the input deck.

Considering the BFP transport in MCNP, there remains a question of how to calculate the exiting energy of an ion after experiencing a within-group transfer (a scattering collision in which the exiting ion remains in the same group). Normally, when a group-to-group transfer event (Boltzmann scatter) occurs, the exiting ion downscatters to a lower group and is given an energy chosen randomly within the new group. Currently, for within-group scattering in MCNP, the same rule applies; the exiting ion is given an energy chosen randomly within the group which may be greater than the energy before the event. However, reference [2] describes a Monte Carlo method for solving the BFP equation where the energy of an ion is not changed after a within-group transfer. Both of these treatments for within-group scattering were tested for 100 keV gold incident on gold with no apparent effect on the deposition profiles. It is uncertain why MCNP chooses a new energy for within-group transfers, but it has been suggested that this could serve as a straggling effect. Within-group transfers are rare along the history of a particle except at low energies (or higher numbered groups). It should also be noted that for ions, the probability of within-group scattering is in general much greater than that for electrons.

The output for multigroup transport in MCNP is formatted for neutrons. It might be convenient to modify the output of MCNP to better accommodate BFP ion transport results, although this is not currently done with multigroup electron/photon problems.

7 Results

The results are in the form of ion deposition profiles from MCNP co-plotted with TRIM profiles. In most cases there are 50 bins evenly spaced for the MCNP simulations, and 100 evenly spaced bins for TRIM. Straight lines are drawn to connect the data points and the plots are presented as continuous curves. The number of histories used to make each plot varies, but most show data from 1×10^6 histories. The attached figures include:

Figure 2a: 100 keV Au \rightarrow Au

Figure 2b: 1 MeV Au \rightarrow Au

Figure 2c: 100 keV Si \rightarrow Si

Figure 2d: 10 keV B \rightarrow Si

Figure 2e: 180 keV As \rightarrow Si

For the two gold incident on gold plots (Figures 2a and 2b), the results from MCNP give a curve that appears to be uniformly shifted to the left of the TRIM curve, which

would indicate that the ions are being deposited at a shallower depth than those simulated with TRIM. For boron incident on silicon (Figure 2c) and silicon incident on silicon (Figure 2d), the results from MCNP show a more “spread out” distribution than that of TRIM, with fewer ions being deposited at the peak of the deposition range. Figure 2e shows the deposition curve from MCNP simulations of arsenic incident on silicon, where the agreement is the worst of the plots made so far. The curve is largely shifted to the right, indicating that the ions are traveling much farther into the material than is predicted with TRIM. The differences in the curves are not presently understood. However, the differences between results from MCNP and TRIM do not appear to be systematic and it is hoped to compare the curves with experimental data.

7.1 Sensitivity Notes

After running many MCNP simulations with various changes in input parameters, several lessons were learned. The following notes on the sensitivity of the deposition profile to various input parameters are primarily based on 100 keV gold incident on gold. In general, the results seem to “converge” to one profile.

Number of Groups: It appears that the number of groups is one of the most important input parameters to YATC. A simulation with too few groups results in a poor deposition profile. Choosing the number of groups for a particular problem is currently done by trial and error. Figure 2b shows the effect of increasing the number of groups from 101 to 201. The curve from the MCNP simulation is slightly shifted to the right, but the effect is small and it is concluded that the curve is converged using 101 groups.

Group Structure: Certainly it is necessary to use a log group structure as it would require a very large number of groups to adequately represent the lower energy groups using a linear group structure. The effect of the additional small energy group (group 1) has not been fully tested.

Legendre Order: It is important that the Legendre order be high enough so that the P0 cross sections are all positive. For 100 keV gold on gold, there was no difference in the results using P9, P11, or P15.

PRF cutoff μ_{cut} : Surprisingly, it appears that the deposition profile is not very sensitive to μ_{cut} . This effect has been tested for several ion-target pairs. For boron incident on silicon, there was only a small difference in the curves for μ_{cut} values of 0.75 and 0.90 as is shown in Figure 2c.

Lowest Energy in group structure: The lowest energy for the cross-section data should be chosen so that an ion with this energy for the ion-target pair under consideration will travel a negligible distance.

YATC tolerance: There are cases where the tolerance for the adaptive quadrature integrals is sufficient for some group-to-group transfer and not for others. All P0 group-to-group transfers should be positive. A sufficient tolerance is currently found by trial and error.

8 Future Work

For coupled multigroup electron/photon problems, the CEPXS code is used to generate the cross sections for MCNP. When the BFP transport of these coupled electron/photon problems was tested in MCNP, it was primarily the energy deposition results that were compared with other data. The results showed very good agreement. Energy deposition comparisons have yet to be made with YATC/MCNP. A top priority right now is obtaining energy deposition profiles with MCNP and comparing with results from TRIM.

One of the principle reasons for wanting to use MCNP with charged particles is the potential to accurately perform truly multidimensional ion transport calculations in amorphous media, with applications in the microelectronics industry. Once the results for single species problems discussed in this memo are satisfactory, the natural step is to test 2D and 3D models. Particularly desirable is the ability to calculate implantation and radiation damage profiles in semiconductor materials of complex geometry for a variety of implant conditions (e.g. incident ion type, energy, and direction).

We would like to soon compare results from MCNP and TRIM with experimental data and ONEBFP results when available. Comparing results with ONEBFP will be a good test of the methods used for transport, as the cross-section data will essentially be the same.

CEPXS can create multigroup electron-only cross-section data. However, no known benchmarks have been performed using multigroup electron-only data in MCNP. This type of calculation (electron-only) would be very similar to the runs performed with ions. We would like to find a problem in which electron-only transport is appropriate, and use MCNP to test the electron-only cross-section data.

Currently, YATC uses an accepted approximation to the scattering integral[9] which is included in the equation for the differential scattering cross section. We would like to explore other approximations or calculations that might prove to be more accurate.

There is ongoing research being done with creating data for the transport of recoil atoms (or ions). Since MCNP currently has the capability to handle more than one multigroup species (coupled electron-photon problems, for example), it is hoped that the group-to-group transfer tables for multiple ion-target pairs can be modelled with little modification to the MCNP code. This ability would have a wide range of applications including radiation damage studies of materials in nuclear reactors, radioactive waste encapsulation, spacecraft component integrity, space shielding, and radiation therapy applications [19, 20, 21].

References

- [1] Briemeister, J.F. (ed.), *MCNPTM - A General Monte Carlo N-Particle Code, Version 4A*, Los Alamos National Laboratory Manual LA-12625-M, 1993.
- [2] Morel, J.E., and Lorence Jr., L.J., et al., *A Hybrid Multigroup/Continuous-Energy Monte Carlo Method for Solving the Boltzmann-Fokker-Planck Equation*, Nuclear Science and Engineering, 124:369-389, 1996.
- [3] Lorence, Jr., L.J., Morel, J.E., Valdez, G.D., *Physics Guide to CEPXS: A Multigroup Coupled Electron-Photon Cross-Section Generating Code*. Technical Report, Sandia National Laboratories, Sandia Report SAND89-1685, 1989.
- [4] Ziegler, James F., *SRIM: The Stopping and Range of Ions in Matter* Instruction Manual, 1996.
- [5] Vandeburg, J.W., Warsa, J.S., Prinja, A.K., *Cross Sections for Ion Transport in the Fokker-Planck Formalism*, American Nuclear Society Transactions, Philadelphia Meeting, June 1995.
- [6] Brasure, Wayne, L., *A Boltzmann Fokker-Planck Decomposition Scheme for Highly Forward-Peaked Ion Cross Sections*, Dissertation, University of New Mexico, 1991.
- [7] Warsa, Jim, Personal Communications, University of New Mexico, 1996.
- [8] Lehmann, C., **Interaction of Radiation with Solids and Elementary Defect Production**, North-Holland Publishing Co., Amsterdam, 1977.
- [9] Ziegler J.F., Biersack, J.P., and Littmark, U., **The Stopping Power and Range of Ions in Solids – Volume I**. Pergamon Press, New York, 1985.
- [10] Morel, J.E., *Fokker-Planck Calculations Using Standard Discrete Ordinates Transport Codes*, Nuclear Science and Engineering, 79:340-356, 1981.
- [11] Przybylski K. and Ligou J., *Numerical Analysis of the Boltzmann Equation Including Fokker-Planck Terms*, Nuclear Science and Engineering, 81:92-109, 1982.
- [12] Landesman, Mark and Morel, J.E., *Angular Fokker-Planck Decomposition and Representation Techniques*, Nuclear Science and Engineering, 103:1-11, 1989.
- [13] Sloan, Daniel, *A New Multigroup Monte Carlo Scattering Algorithm Suitable for Neutral and Charged-Particle Boltzmann and Fokker-Planck Calculations*, Dissertation, University of New Mexico, 1983.
- [14] Wagner, J.C., Redmond II, E.L., et al., *MCNP: Multigroup/Adjoint Capabilities* Technical Report, Los Alamos National Laboratory, LANL Report LA-12704, 1994.

- [15] Adams, Ken, Personal Communication, Los Alamos National Laboratory, XTM, 1996.
- [16] Little, Bob, Personal Communication, Los Alamos National Laboratory, XTM, 1996.
- [17] Hart, Michelle, *Depth Dose in Aluminum and Physics Documentation of MCNP Multi-group Subroutines*, Los Alamos National Laboratory, XTM memorandum, XTM:95-235, 1995.
- [18] Van Riper, Kenneth A., *Sabrina User's Guide*, Los Alamos National Laboratory Report LA-UR-93-3696, 1994.
- [19] Robertson, J.A.L., **Irradiation Effects in Nuclear Fuels**, Gordon and Breach, U.S.A. (A.E.C Monograph), 1969.
- [20] Arnold, G.W., *Ion Implantation Damage Process in Nuclear Waste Glass and other Silicate Glass*, Materials Research Society Symposium Proceedings, 44, p. 617, 1986.
- [21] Rester, A.C., and Trombka, J. (eds.), *High-Energy Radiation Background in Space*, AIP Conference Proceedings 186, Florida, 1987.

A Example of input to YATC (input)

```

LEGENDRE-ORDER 5
! energy in keV
ION-PAIRS 1
ENERGY-BASIS-ORDER 1           ! only step implemented for now
ENERGY-GRID-TYPE log 4
ENERGY-GRID
    100.0 1.0
PAIR au->au
    PRF-ORDER 5
    SCREENING-FUNCTION 3
    PRF-CUTOFF 0.90
TOLERANCE 1.0e-2
CONTROL
    DoGroupTransfers    1
    DoOnlyPO             0
    DoMomentumTransfer  1
    DoStoppingPower      1
    PrintInfo            1
    PlotStoppingPowers   0

```

B Example of input to CRSRD (crsrd.inp)

```

yout.dtf    DTF
type1 = ace.out

```

```

iskip =    0
ilen =    9
itpos =    5
ispos =    6
ibfp = 1
i2lp1 = 0
ititl = 2
iengb = 1
iincp = 1    4 0
iball = 0
nabs = 1
iprocc = 1
ipn = 5
iang = 2
energy
1.00000E-01 3.16228E-02 1.00000E-02 3.16228E-03 1.00000E-03
1.83475E+05 1.83475E+05 1.83475E+05 1.83475E+05
materials
79197.01    196.9665400
nutotal
end

```

C Example of DTF-formatted data (yout.dtf)

```

legendre order: 0    total energy groups: 4
4.69735E+04 1.15474E+04 1.34595E+04 0.00000E+00 5.98966E+06 4.99112E+06
0.00000E+00 0.00000E+00 0.00000E+00 8.47537E+04 6.67819E+03 9.80607E+04
0.00000E+00 1.21648E+07 1.00618E+07 8.43275E+05 0.00000E+00 0.00000E+00
1.42584E+05 3.72904E+03 6.81531E+05 0.00000E+00 2.24510E+07 1.84541E+07
1.75846E+06 1.11346E+05 0.00000E+00 2.27257E+05 2.03453E+03 7.12953E+06
0.00000E+00 3.86030E+07 3.14735E+07 3.31533E+06 2.46497E+05 3.04683E+04
legendre order: 1    total energy groups: 4
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 4.70948E+06
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
0.00000E+00 0.00000E+00 9.46910E+06 6.39953E+05 0.00000E+00 0.00000E+00
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 1.73288E+07
1.31553E+06 4.05911E+04 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
0.00000E+00 0.00000E+00 2.95016E+07 2.45134E+06 8.92600E+04 6.15224E+03
legendre order: 2    total energy groups: 4
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 4.20461E+06
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
0.00000E+00 0.00000E+00 8.41025E+06 3.38994E+05 0.00000E+00 0.00000E+00
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 1.53241E+07
6.64729E+05-3.23789E+04 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
0.00000E+00 0.00000E+00 2.59965E+07 1.19079E+06-7.23386E+04-1.32780E+04
legendre order: 3    total energy groups: 4
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 3.57268E+06

```

```

0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
0.00000E+00 0.00000E+00 7.09851E+06 7.37009E+04 0.00000E+00 0.00000E+00
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 1.28426E+07
1.06558E+05-4.53769E+04 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
0.00000E+00 0.00000E+00 2.16751E+07 1.30203E+05-1.00179E+05-8.50628E+03
  legendre order: 4   total energy groups: 4
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 2.91548E+06
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
0.00000E+00 0.00000E+00 5.73626E+06-5.88920E+04 0.00000E+00 0.00000E+00
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 1.03121E+07
-1.57780E+05-5.21882E+03 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
0.00000E+00 0.00000E+00 1.72948E+07-3.46887E+05-1.04783E+04 6.82628E+03
  legendre order: 5   total energy groups: 4
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 2.31485E+06
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
0.00000E+00 0.00000E+00 4.51154E+06-7.68823E+04 0.00000E+00 0.00000E+00
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 8.04243E+06
-1.69962E+05 3.05154E+04 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
0.00000E+00 0.00000E+00 1.34127E+07-3.31098E+05 6.80966E+04 9.13292E+03

```

D Example of output from YATC (yout)

```

Incident charge and mass: 7.90000E+01 1.96967E+02
Target charge and mass: 7.90000E+01 1.96967E+02

```

```

Recoils?      F
  mu_cut =    0.90000
    PRF =     5
      L =     5
  USF index =  3
global tol =  1.00000E-02

```

4 Energy Group(s) (keV):

```

1.0000000000E+02 3.1622776602E+01 1.0000000000E+01 3.1622776602E+00
1.0000000000E+00

```

Upper	Lower	Midpoint	Width
1.00000E+02	3.16228E+01	5.62341E+01	6.83772E+01
3.16228E+01	1.00000E+01	1.77828E+01	2.16228E+01
1.00000E+01	3.16228E+00	5.62341E+00	6.83772E+00
3.16228E+00	1.00000E+00	1.77828E+00	2.16228E+00

```

number groups = 4
density = 19.320000000000000 g/cm^3
target mass = 196.966540000000009 amu
atom density (N) = 0.590697694359661230E+23

```

Group-to-Group Transfers:

units are 1/cm

legendre order: 0

```
big_sigma( 1--> 1) =      4.99111593E+06
big_sigma( 1--> 2) =      8.43274695E+05
big_sigma( 1--> 3) =      1.11346284E+05
big_sigma( 1--> 4) =      3.04682575E+04
big_sigma( 2--> 1) =      0.00000000E+00
big_sigma( 2--> 2) =      1.00617514E+07
big_sigma( 2--> 3) =      1.75845917E+06
big_sigma( 2--> 4) =      2.46497170E+05
big_sigma( 3--> 1) =      0.00000000E+00
big_sigma( 3--> 2) =      0.00000000E+00
big_sigma( 3--> 3) =      1.84541149E+07
big_sigma( 3--> 4) =      3.31533286E+06
big_sigma( 4--> 1) =      0.00000000E+00
big_sigma( 4--> 2) =      0.00000000E+00
big_sigma( 4--> 3) =      0.00000000E+00
big_sigma( 4--> 4) =      3.14734935E+07
```

momentum transfer(alpha) and stopping power

```
group: 1 -----
alpha =      7.95220825E-19 [cm^2]      4.69735108E+04 [1/cm]
yatc nuclear SP      9.87085342E-17 [keV*cm^2]      5.83069035E+03 [MeV/cm]
electronic SP =      9.67791284E-17 [keV*cm^2]      5.71672080E+03 [MeV/cm]
total stopping =      1.95487663E-16 [keV*cm^2]      1.15474112E+04 [MeV/cm]
group: 2 -----
alpha =      1.43480723E-18 [cm^2]      8.47537324E+04 [1/cm]
yatc nuclear SP      5.67205784E-17 [keV*cm^2]      3.35047149E+03 [MeV/cm]
electronic SP =      5.63354420E-17 [keV*cm^2]      3.32772157E+03 [MeV/cm]
total stopping =      1.13056020E-16 [keV*cm^2]      6.67819306E+03 [MeV/cm]
group: 3 -----
alpha =      2.41382366E-18 [cm^2]      1.42584007E+05 [1/cm]
yatc nuclear SP      3.03364190E-17 [keV*cm^2]      1.79196527E+03 [MeV/cm]
electronic SP =      3.27930421E-17 [keV*cm^2]      1.93707743E+03 [MeV/cm]
total stopping =      6.31294611E-17 [keV*cm^2]      3.72904271E+03 [MeV/cm]
group: 4 -----
alpha =      3.84726037E-18 [cm^2]      2.27256783E+05 [1/cm]
yatc nuclear SP      1.53539256E-17 [keV*cm^2]      9.06952843E+02 [MeV/cm]
electronic SP =      1.90889353E-17 [keV*cm^2]      1.12757901E+03 [MeV/cm]
total stopping =      3.44428609E-17 [keV*cm^2]      2.03453185E+03 [MeV/cm]
```

Total and Absorption cross sections:

```
group 1 tot: 5.98966E+06 abs: 1.34595E+04
group 2 tot: 1.21648E+07 abs: 9.80607E+04
group 3 tot: 2.24510E+07 abs: 6.81531E+05
```

group 4 tot: 3.86030E+07 abs: 7.12953E+06

number calls to USF function = 2.26315E+06

E Example of ACE-formatted data (ace.out)

79197.01m195.274487

11/12/96

137	79197	7	3	4	0	3	0
1	0	1	0	0	0	0	0
1	13	0	0	0	17	21	25
29	32	0	0	44	0	0	55
56	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0

6.58114000000000E-02 2.08114000000000E-02 6.58114000000000E-03 2.08114000000000E-03
6.83772000000000E-02 2.16228000000000E-02 6.83772000000000E-03 2.16228000000000E-03
1.83475000000000E+05 1.83475000000000E+05 1.83475000000000E+05 1.83475000000000E+05
5.98966000000000E+06 1.21648000000000E+07 2.24510000000000E+07 3.86030000000000E+07
1.34595000000000E+04 9.80607000000000E+04 6.81531000000000E+05 7.12953000000000E+06
1.15474000000000E+04 6.67819000000000E+03 3.72904000000000E+03 2.03453000000000E+03
4.69735000000000E+04 8.47537000000000E+04 1.42584000000000E+05 2.27257000000000E+05
1.00000000000000E+00 9.04000000000000E+02 9.05000000000000E+02 5.98966000000000E+06
1.21648000000000E+07 2.24510000000000E+07 3.86030000000000E+07 5.97620930000000E+06
1.20667570000000E+07 2.17694300000000E+07 3.14735000000000E+07 1.34595000000000E+04
9.80607000000000E+04 6.81531000000000E+05 7.12953000000000E+06 4.50000000000000E+01
4.99112000000000E+06 8.43275000000000E+05 1.11346000000000E+05 3.04683000000000E+04
1.00618000000000E+07 1.75846000000000E+06 2.46497000000000E+05 1.84541000000000E+07
3.31533000000000E+06 3.14735000000000E+07 5.70000000000000E+01 6.70000000000000E+01
1.00000000000000E+00 8.00000000000000E+00 1.50000000000000E+01 2.20000000000000E+01
2.90000000000000E+01 3.60000000000000E+01 4.30000000000000E+01 5.00000000000000E+01
5.70000000000000E+01 6.40000000000000E+01 1.00000000000000E+00 1.00000000000000E+00
1.00000000000000E+00 9.4357178348747E-01 .00000000000000E+00 .00000000000000E+00
.00000000000000E+00 7.5018568092907E-01 9.9115448311293E-01 1.00000000000000E+00
6.9274428688445E-01 1.00000000000000E+00 -1.9960449696968E-01 .00000000000000E+00
5.5597587513960E-01 9.9856215979712E-01 9.9985486934086E-01 2.9401818728160E-01
4.5409236973612E-01 -2.9365879209224E-02 1.00000000000000E+00 6.0680386015415E-01
9.9781561453703E-01 9.9999833118369E-01 1.6717369679069E-01 2.5707534847179E-01
-1.8390991143447E-02 1.00000000000000E+00 1.00000000000000E+00 1.00000000000000E+00
1.00000000000000E+00 9.4109403883997E-01 .00000000000000E+00 .00000000000000E+00
.00000000000000E+00 7.6076266706215E-01 9.8228394863908E-01 1.00000000000000E+00
6.9153236705857E-01 1.00000000000000E+00 2.8309821222540E-02 .00000000000000E+00
5.6157308143603E-01 9.9853305738820E-01 9.9985455294915E-01 2.9247168588211E-01
4.5258938747698E-01 -2.9648421831602E-02 1.00000000000000E+00 1.00000000000000E+00

```

1.000000000000000E+00 1.000000000000000E+00 9.3902168081890E-01 .000000000000000E+00
.000000000000000E+00 .000000000000000E+00 7.6670017348731E-01 9.7522239081666E-01
1.000000000000000E+00 6.8901938141136E-01 1.000000000000000E+00 1.0501329435976E-01
.000000000000000E+00 1.000000000000000E+00 1.000000000000000E+00 1.000000000000000E+00
9.3734729216643E-01 .000000000000000E+00 .000000000000000E+00 .000000000000000E+00
.000000000000000E+00

```

F Example of output from READMG (info)

zaid= 79197.01m

atomic weight: 1.95274E+02

energy MeV: 0.00000E+00

date of processing: 11/12/96

comment:

material:

```

nxs( 1) LDB, length of second data block: 137
nxs( 2) ZA, 1000*Z+A -- ZAID: 79197
nxs( 3) NLEG, # of angular dist variables: 7
nxs( 4) NEDIT, number of edit reactions: 3
nxs( 5) NGRP, number of groups: 4
nxs( 6) NUS, number of upscatter groups: 0
nxs( 7) NDS, # of downscatter groups: 3
nxs( 8) NSEC, # of secondary particles: 0
nxs( 9) ISANG, angular distribution type: 1 discrete cosines
nxs(10) NNUBAR, number of nubars given: 0
nxs(11) IBFP,boltz-fokker-plank indicator: 1 BFP treatment
nxs(12) IPT, incident particle: 0 other particle
sum of nxs(13) thru nxs(16) (not used): 0

```

```

jxs( 1) LERG, inc. part. group struct.: 1
jxs( 2) LTOT, total cross sections: 13
jxs( 3) LFISS, fission cross sections: 0
jxs( 4) LNU, nubar data: 0
jxs( 5) LCHI, fission chi data: 0
jxs( 6) LABS, absorption cross section: 17
jxs( 7) LSTOP, stopping powers: 21
jxs( 8) LMOM, momentum transfer: 25
jxs( 9) LMTED, edit reaction numbers: 29
jxs(10) LXSED, edit cross sections: 32
jxs(11) LIPT, secondary particles: 0
jxs(12) LERG2L, sec. group struct. loc.: 0
jxs(13) LPOL, PO locators: 44
jxs(14) LSANG2, sec. angular dist. types: 0
jxs(15) LNLEG2, # of ang dist var for sec: 0
jxs(16) LXPNL, XPN locators: 55
jxs(17) LPNL, PN locators: 56

```

sum of jxs(18) thru nxs(32) (not used): 0

energy boundaries for incident particle ngroups= 4

group	upper energy	lower energy	center energy	energy width
1	1.0000E-01	3.1623E-02	6.5811E-02	6.8377E-02
2	3.1623E-02	1.0000E-02	2.0811E-02	2.1623E-02
3	1.0000E-02	3.1623E-03	6.5811E-03	6.8377E-03
4	3.1623E-03	1.0000E-03	2.0811E-03	2.1623E-03

group masses(mev)

1	1.83475E+05
2	1.83475E+05
3	1.83475E+05
4	1.83475E+05

number of particles= 1
particle number 1 is group 1 through 4

group	sigtot	sigabs	stop power	mom transf
1	5.98966E+06	1.34595E+04	1.15474E+04	4.69735E+04
2	1.21648E+07	9.80607E+04	6.67819E+03	8.47537E+04
3	2.24510E+07	6.81531E+05	3.72904E+03	1.42584E+05
4	3.86030E+07	7.12953E+06	2.03453E+03	2.27257E+05

group	mt= 1	mt= 904	mt= 905
1	5.98966E+06	5.97621E+06	1.34595E+04
2	1.21648E+07	1.20668E+07	9.80607E+04
3	2.24510E+07	2.17694E+07	6.81531E+05
4	3.86030E+07	3.14735E+07	7.12953E+06

G Example of READMG output (p0)

pssc0 matrix for incident particle

s(1-> 1)= 4.99112E+06 s(1-> 2)= 8.43275E+05 s(1-> 3)= 1.11346E+05
s(1-> 4)= 3.04683E+04
sum to particle 1 is 5.97621E+06 multiplicity= 9.97754E-01

s(2-> 2)= 1.00618E+07 s(2-> 3)= 1.75846E+06 s(2-> 4)= 2.46497E+05
sum to particle 1 is 1.20668E+07 multiplicity= 9.91940E-01

s(3-> 3)= 1.84541E+07 s(3-> 4)= 3.31533E+06
sum to particle 1 is 2.17694E+07 multiplicity= 9.69642E-01

s(4-> 4)= 3.14735E+07
sum to particle 1 is 3.14735E+07 multiplicity= 8.15312E-01

H Example of READMG output (cosines)

```

      pscn matrix for incident particle
      there are 7 values in the pscn array
for group 1 to group 1:
  1.0000E+00  1.0000E+00  1.0000E+00  9.4357E-01  0.0000E+00  0.0000E+00
  0.0000E+00
for group 1 to group 2:
  7.5019E-01  9.9115E-01  1.0000E+00  6.9274E-01  1.0000E+00 -1.9960E-01
  0.0000E+00
for group 1 to group 3:
  5.5598E-01  9.9856E-01  9.9985E-01  2.9402E-01  4.5409E-01 -2.9366E-02
  1.0000E+00
for group 1 to group 4:
  6.0680E-01  9.9782E-01  1.0000E+00  1.6717E-01  2.5708E-01 -1.8391E-02
  1.0000E+00
for group 2 to group 2:
  1.0000E+00  1.0000E+00  1.0000E+00  9.4109E-01  0.0000E+00  0.0000E+00
  0.0000E+00
for group 2 to group 3:
  7.6076E-01  9.8228E-01  1.0000E+00  6.9153E-01  1.0000E+00  2.8310E-02
  0.0000E+00
for group 2 to group 4:
  5.6157E-01  9.9853E-01  9.9985E-01  2.9247E-01  4.5259E-01 -2.9648E-02
  1.0000E+00
for group 3 to group 3:
  1.0000E+00  1.0000E+00  1.0000E+00  9.3902E-01  0.0000E+00  0.0000E+00
  0.0000E+00
for group 3 to group 4:
  7.6670E-01  9.7522E-01  1.0000E+00  6.8902E-01  1.0000E+00  1.0501E-01
  0.0000E+00
for group 4 to group 4:
  1.0000E+00  1.0000E+00  1.0000E+00  9.3735E-01  0.0000E+00  0.0000E+00
  0.0000E+00

```

I Example of input to MCNP (inp)

```

slab : gold on gold test
1001 0          3000 -1 -2000  imp:n=1
      1 1 1.0    1 -2 -2000  imp:n=1
      2 1 1.0    2 -3 -2000  imp:n=1
      3 1 1.0    3 -4 -2000  imp:n=1
      4 1 1.0    4 -5 -2000  imp:n=1
      5 1 1.0    5 -6 -2000  imp:n=1
      6 1 1.0    6 -7 -2000  imp:n=1
      7 1 1.0    7 -8 -2000  imp:n=1
      8 1 1.0    8 -9 -2000  imp:n=1

```

9	1	1.0	9	-10	-2000	imp:n=1
10	1	1.0	10	-11	-2000	imp:n=1
11	1	1.0	11	-12	-2000	imp:n=1
12	1	1.0	12	-13	-2000	imp:n=1
13	1	1.0	13	-14	-2000	imp:n=1
14	1	1.0	14	-15	-2000	imp:n=1
15	1	1.0	15	-16	-2000	imp:n=1
16	1	1.0	16	-17	-2000	imp:n=1
17	1	1.0	17	-18	-2000	imp:n=1
18	1	1.0	18	-19	-2000	imp:n=1
19	1	1.0	19	-20	-2000	imp:n=1
20	1	1.0	20	-21	-2000	imp:n=1
21	1	1.0	21	-22	-2000	imp:n=1
22	1	1.0	22	-23	-2000	imp:n=1
23	1	1.0	23	-24	-2000	imp:n=1
24	1	1.0	24	-25	-2000	imp:n=1
25	1	1.0	25	-26	-2000	imp:n=1
26	1	1.0	26	-27	-2000	imp:n=1
27	1	1.0	27	-28	-2000	imp:n=1
28	1	1.0	28	-29	-2000	imp:n=1
29	1	1.0	29	-30	-2000	imp:n=1
30	1	1.0	30	-31	-2000	imp:n=1
31	1	1.0	31	-32	-2000	imp:n=1
32	1	1.0	32	-33	-2000	imp:n=1
33	1	1.0	33	-34	-2000	imp:n=1
34	1	1.0	34	-35	-2000	imp:n=1
35	1	1.0	35	-36	-2000	imp:n=1
36	1	1.0	36	-37	-2000	imp:n=1
37	1	1.0	37	-38	-2000	imp:n=1
38	1	1.0	38	-39	-2000	imp:n=1
39	1	1.0	39	-40	-2000	imp:n=1
40	1	1.0	40	-41	-2000	imp:n=1
41	1	1.0	41	-42	-2000	imp:n=1
42	1	1.0	42	-43	-2000	imp:n=1
43	1	1.0	43	-44	-2000	imp:n=1
44	1	1.0	44	-45	-2000	imp:n=1
45	1	1.0	45	-46	-2000	imp:n=1
46	1	1.0	46	-47	-2000	imp:n=1
47	1	1.0	47	-48	-2000	imp:n=1
48	1	1.0	48	-49	-2000	imp:n=1
49	1	1.0	49	-50	-2000	imp:n=1
50	1	1.0	50	-51	-2000	imp:n=1
1002	0	2000:-3000:	51			imp:n=0
2000	cx	1.0E-04				
3000	px	-1000.E-08				
1	px	0.00000000E+00				

2	px	5.00000000E-08
3	px	1.00000000E-07
4	px	1.50000000E-07
5	px	2.00000000E-07
6	px	2.50000000E-07
7	px	3.00000000E-07
8	px	3.50000000E-07
9	px	4.00000000E-07
10	px	4.50000000E-07
11	px	5.00000000E-07
12	px	5.50000000E-07
13	px	6.00000000E-07
14	px	6.50000000E-07
15	px	7.00000000E-07
16	px	7.50000000E-07
17	px	8.00000000E-07
18	px	8.50000000E-07
19	px	9.00000000E-07
20	px	9.50000000E-07
21	px	1.00000000E-06
22	px	1.05000000E-06
23	px	1.10000000E-06
24	px	1.15000000E-06
25	px	1.20000000E-06
26	px	1.25000000E-06
27	px	1.30000000E-06
28	px	1.35000000E-06
29	px	1.40000000E-06
30	px	1.45000000E-06
31	px	1.50000000E-06
32	px	1.55000000E-06
33	px	1.60000000E-06
34	px	1.65000000E-06
35	px	1.70000000E-06
36	px	1.75000000E-06
37	px	1.80000000E-06
38	px	1.85000000E-06
39	px	1.90000000E-06
40	px	1.95000000E-06
41	px	2.00000000E-06
42	px	2.20000000E-06
43	px	2.40000000E-06
44	px	2.60000000E-06
45	px	2.80000000E-06
46	px	3.00000000E-06
47	px	3.20000000E-06
48	px	3.40000000E-06

```

49   px   3.60000000E-06
50   px   3.80000000E-06
51   px   4.00000000E-06

sdef erg=1 pos=-10.0e-8  0 0 vec=1 0 0 dir=1.0
mgopt f -4
m1      79197.01m  -1
f1:n 1 49I 51
c0 0 1
cut:n j .001
nps 1e6
print 110 -120 -130 -50 -60 -70 -98 -140
prdmp 2j 1 1
rdum 0.90

```

Notes on Appendices

These files presented in the Appendix are a set of consistent data files for a very small problem (P5, 4 groups). The files were generated solely to be used as examples in this memo and were not intended to be used for a real simulation. The data files that were generated to obtain the results shown in the attached figures are very much larger in file size (about 1 Megabyte for **yout.dtf**).

Figure 1: Legendre Expansion Fits to Cross Section

Au→Au at 10 keV

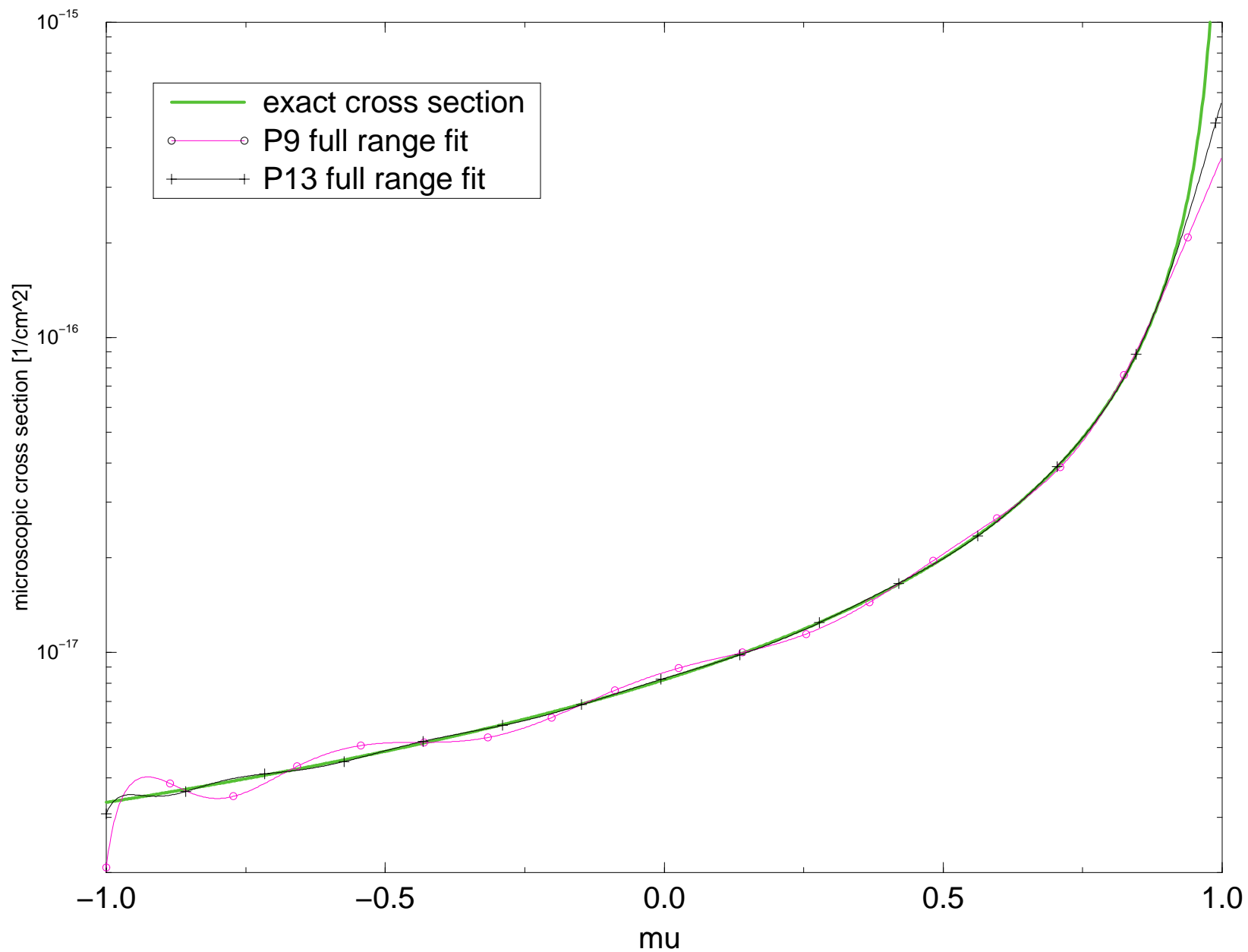


Figure 2a: Au→Au 100 keV Ion Deposition Profile

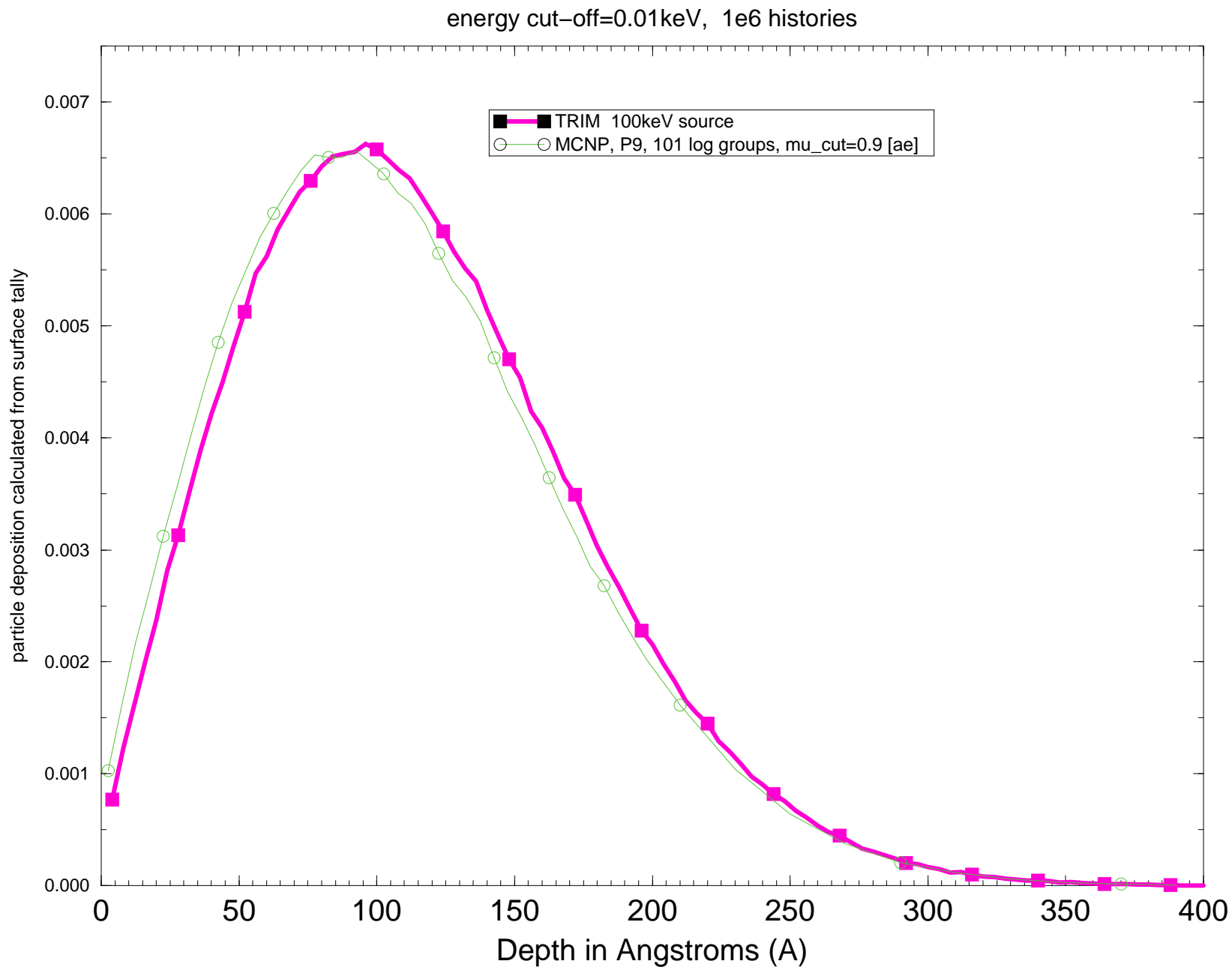


Figure 2b: Au→Au 1 MeV Ion Deposition Profile

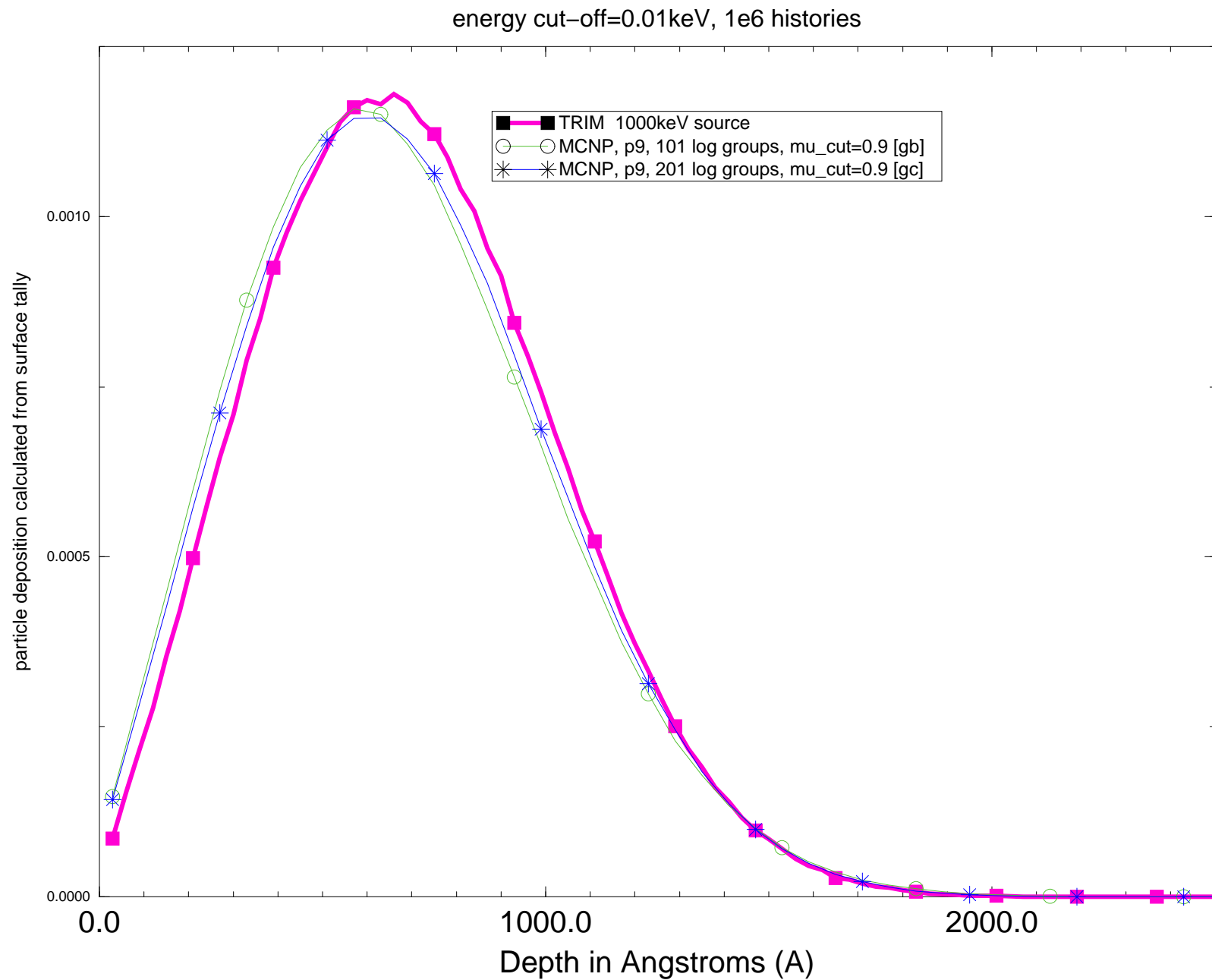


Figure 2c: B→Si 10 keV Ion Deposition Profile

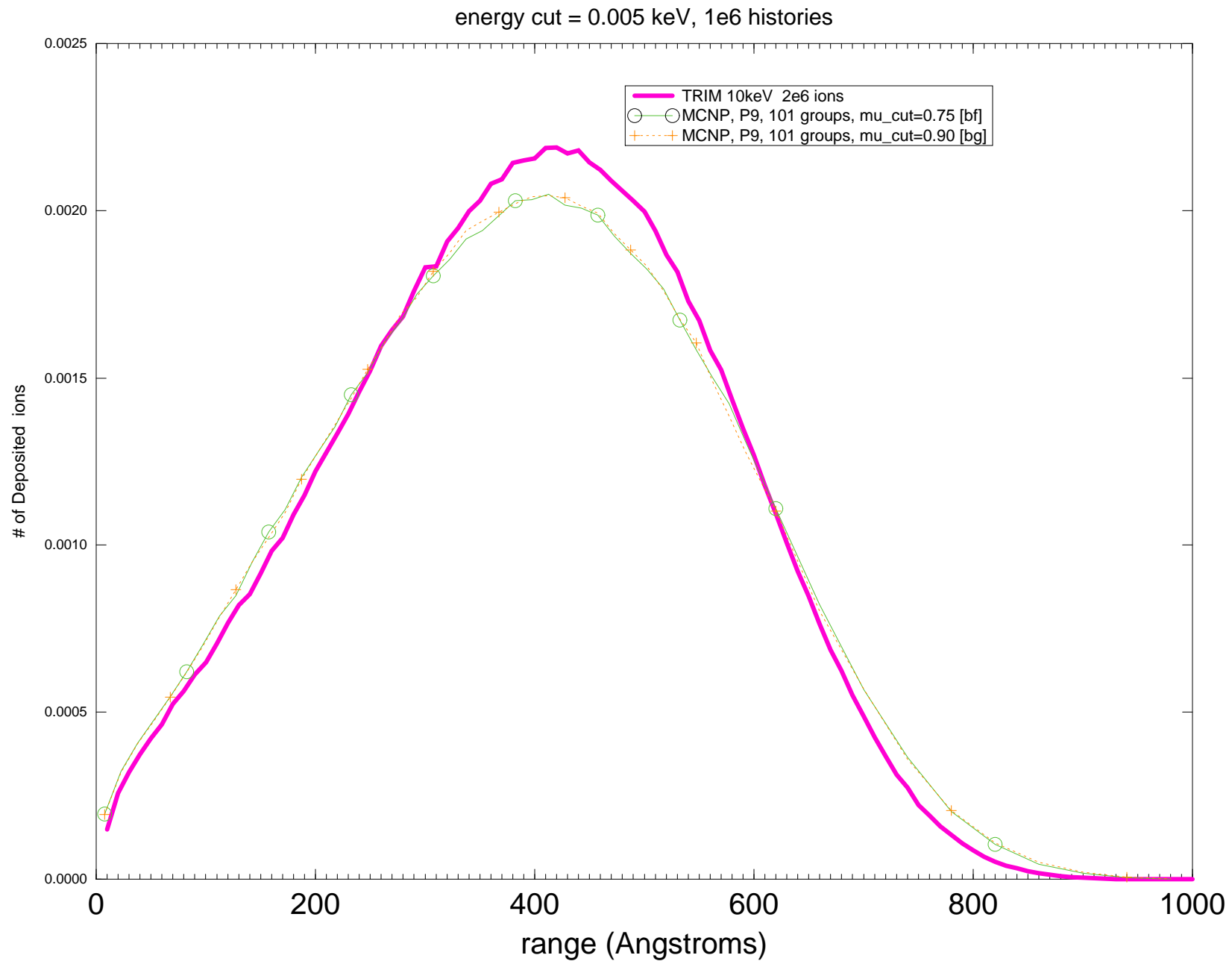


Figure 2d: Si→Si 100 keV Ion Deposition Profile

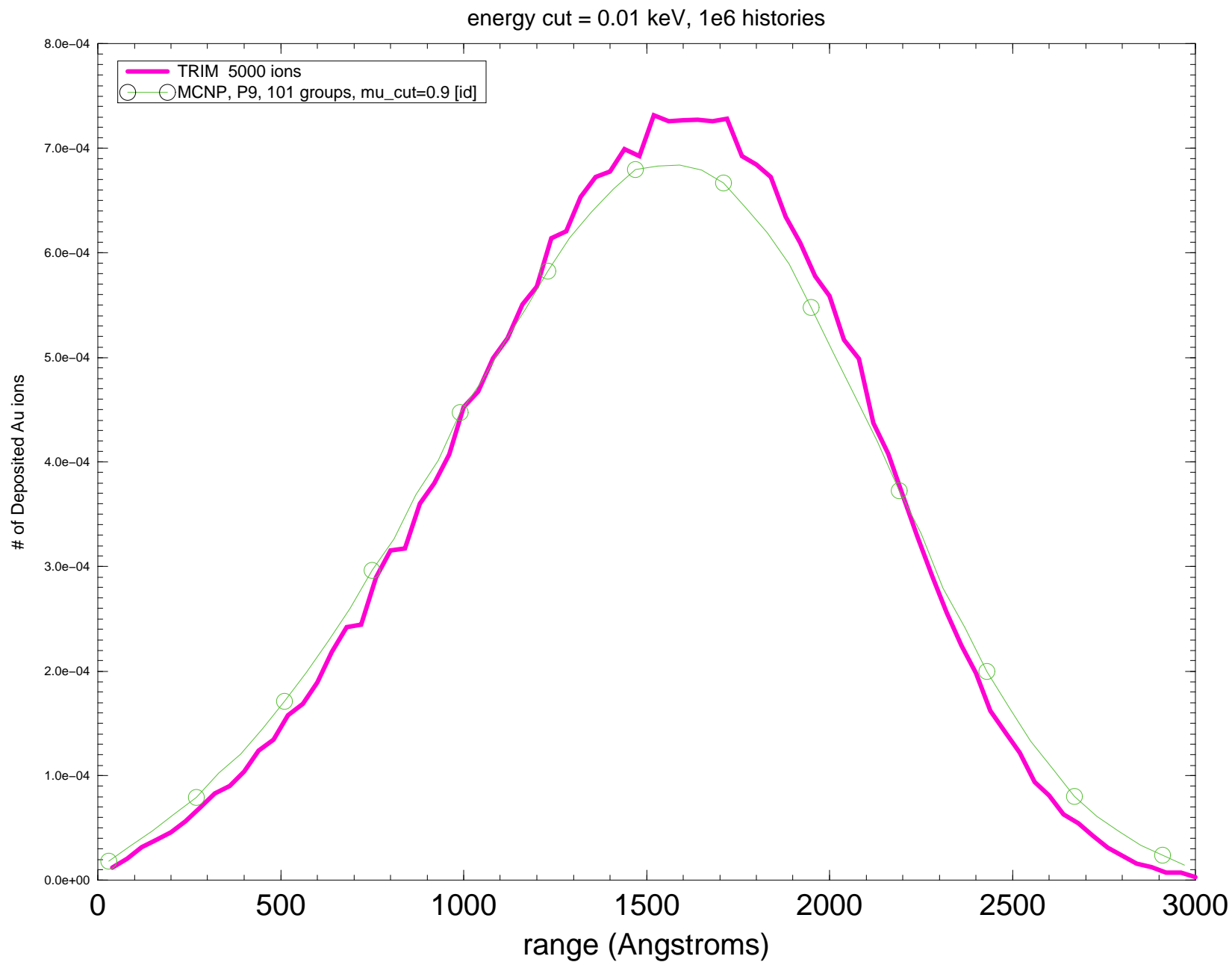


Figure 2e: As→Si 180 keV Ion Deposition Profile

